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LOGINID: SSPTAJRK1626

PASSWORD:

TERMINAL (ENTER 1, 2, 3, OR ?):2

```
Web Page URLs for STN Seminar Schedule - N. America
NEWS 1
                 "Ask CAS" for self-help around the clock
NEWS
     3
NEWS
        DEC 05
                CASREACT(R) - Over 10 million reactions available
                2006 MeSH terms loaded in MEDLINE/LMEDLINE
NEWS
        DEC 14
                2006 MeSH terms loaded for MEDLINE file segment of TOXCENTER
NEWS 5
        DEC 14
NEWS 6 DEC 14 CA/CAplus to be enhanced with updated IPC codes
                IPC search and display fields enhanced in CA/CAplus with the
NEWS 7
        DEC 21
                 IPC reform
                New IPC8 SEARCH, DISPLAY, and SELECT fields in USPATFULL/
NEWS 8
        DEC 23
                 USPAT2
                IPC 8 searching in IFIPAT, IFIUDB, and IFICDB
NEWS 9
        JAN 13
                New IPC 8 SEARCH, DISPLAY, and SELECT enhancements added to
NEWS 10
        JAN 13
                 INPADOC
NEWS 11
        JAN 17
                Pre-1988 INPI data added to MARPAT
                IPC 8 in the WPI family of databases including WPIFV
        JAN 17
NEWS 12
                Saved answer limit increased
        JAN 30
NEWS 13
                Monthly current-awareness alert (SDI) frequency
        JAN 31
NEWS 14
                 added to TULSA
```

NEWS EXPRESS JANUARY 03 CURRENT VERSION FOR WINDOWS IS V8.01,
CURRENT MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP),
AND CURRENT DISCOVER FILE IS DATED 19 DECEMBER 2005.
V8.0 USERS CAN OBTAIN THE UPGRADE TO V8.01 AT
http://download.cas.org/express/v8.0-Discover/

NEWS HOURS STN Operating Hours Plus Help Desk Availability
NEWS INTER General Internet Information
NEWS LOGIN Welcome Banner and News Items
NEWS PHONE Direct Dial and Telecommunication Network Access to STN
NEWS WWW CAS World Wide Web Site (general information)

Enter NEWS followed by the item number or name to see news on that specific topic.

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FILE 'HOME' ENTERED AT 14:42:11 ON 09 FEB 2006

=> file reg
COST IN U.S. DOLLARS

FULL ESTIMATED COST

SINCE FILE TOTAL ENTRY SESSION 0.21 0.21

FILE 'REGISTRY' ENTERED AT 14:42:20 ON 09 FEB 2006
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STRUCTURE FILE UPDATES: 7 FEB 2006 HIGHEST RN 873775-18-9 DICTIONARY FILE UPDATES: 7 FEB 2006 HIGHEST RN 873775-18-9

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH JULY 14, 2005

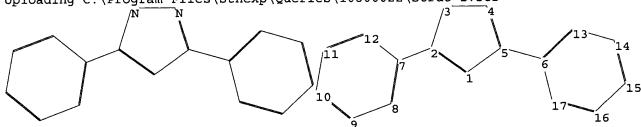
Please note that search-term pricing does apply when conducting SmartSELECT searches.

Structure search iteration limits have been increased. See HELP SLIMITS for details.

REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

http://www.cas.org/ONLINE/UG/regprops.html

=>
Uploading C:\Program Files\Stnexp\Queries\10800022\Struc 1.str



ring nodes :

1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17

chain bonds : 2-7 5-6 ring bonds :

10800022.trn

1-2 1-5 2-3 3-4 4-5 6-13 6-17 7-8 7-12 8-9 9-10 10-11 11-12 13-14

14-15 15-16 16-17 exact/norm bonds :

1-2 1-5 2-3 3-4 4-5

exact bonds: 2-7 5-6

normalized bonds :

6-13 6-17 7-8 7-12 8-9 9-10 10-11 11-12 13-14 14-15 15-16 16-17

Match level :

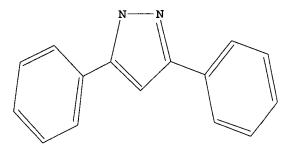
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom

L1 STRUCTURE UPLOADED

=> d

L1 HAS NO ANSWERS

L1 STR



Structure attributes must be viewed using STN Express query preparation.

50 ANSWERS

=> 11

SAMPLE SEARCH INITIATED 14:42:43 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 6344 TO ITERATE

31.5% PROCESSED 2000 ITERATIONS INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**

BATCH **COMPLETE**

PROJECTED ITERATIONS: 122105 TO 131655 PROJECTED ANSWERS: 11296 TO 14332

L2 50 SEA SSS SAM L1

=>

Uploading C:\Program Files\Stnexp\Queries\10800022\Struc 2.str

chain nodes :

18 19
ring nodes :

1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17
chain bonds :

2-7 3-18 5-6 12-19
ring bonds :

1-2 1-5 2-3 3-4 4-5 6-13 6-17 7-8 7-12 8-9 9-10 10-11 11-12 13-14
14-15 15-16 16-17
exact/norm bonds :

1-2 1-5 2-3 3-4 4-5
exact bonds :

2-7 3-18 5-6 12-19
normalized bonds :

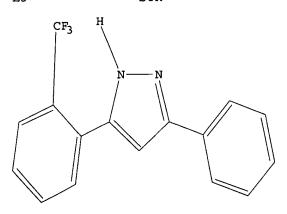
6-13 6-17 7-8 7-12 8-9 9-10 10-11 11-12 13-14 14-15 15-16 16-17

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:CLASS

L3 STRUCTURE UPLOADED

=> d L3 HAS NO ANSWERS L3 STR



Structure attributes must be viewed using STN Express query preparation.

=> 13

SAMPLE SEARCH INITIATED 14:44:15 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 200 TO ITERATE

100.0% PROCESSED 200 ITERATIONS

0 ANSWERS

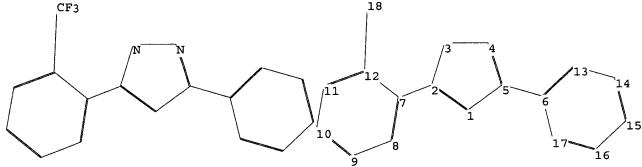
SEARCH TIME: 00.00.02

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 3152 TO 4848
PROJECTED ANSWERS: 0 TO 0

L4

0 SEA SSS SAM L3

=>
Uploading C:\Program Files\Stnexp\Queries\10800022\Struc 3.str



Match level:
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom
11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:CLASS

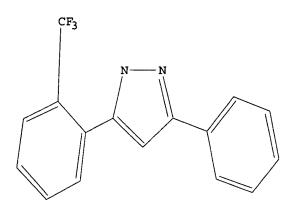
STRUCTURE UPLOADED

L5

=> d

L5 HAS NO ANSWERS

L5 STR



Structure attributes must be viewed using STN Express query preparation.

=> 15

SAMPLE SEARCH INITIATED 14:45:03 FILE 'REGISTRY'

SAMPLE SCREEN SEARCH COMPLETED - 200 TO ITERATE

19 ANSWERS 200 ITERATIONS 100.0% PROCESSED

SEARCH TIME: 00.00.03

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**

PROJECTED ITERATIONS: 3152 TO

PROJECTED ANSWERS: 119 TO 641

L6 19 SEA SSS SAM L5

=> d scan

19 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN L6

Phenol, 3-[1-methyl-5-[2-(trifluoromethyl)phenyl]-1H-pyrazol-3-yl]- (9CI) IN

MF C17 H13 F3 N2 O

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):0

=> 15 full

FULL SEARCH INITIATED 14:45:31 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 4056 TO ITERATE

100.0% PROCESSED 4056 ITERATIONS 322 ANSWERS

SEARCH TIME: 00.00.04

L7 322 SEA SSS FUL L5

=> file medline caplus

COST IN U.S. DOLLARS
SINCE FILE TOTAL
ENTRY SESSION
FULL ESTIMATED COST
169.14
169.35

FILE 'MEDLINE' ENTERED AT 14:45:43 ON 09 FEB 2006

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=> 17 L8 1 L7

=> d ibib abs

L8 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2004:780671 CAPLUS

DOCUMENT NUMBER: 141:296010

TITLE: Preparation of substituted pyrazoles as modulators of

ATP-binding cassette transporters

INVENTOR(S): Vangoor, Frederick F.; Hadida Ruah, Sarah S.; Singh,

Ashvani K.; Olson, Eric R.; Makings, Lewis R.; Gonzalez, Jesus E., III; Rader, James A.; Chambers, Fred, III; Miller, Mark T.; Grootenhuis, Peter; Liu,

Yahua

PATENT ASSIGNEE(S): Vertex Pharmaceuticals Incorporated, USA

SOURCE: PCT Int. Appl., 174 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND DATE	APPLICATION NO.	DATE
WO 2004080972	A1 20040923	WO 2004-US7492	20040312
W: AE, AG, A	, AM, AT, AU, AZ,	BA, BB, BG, BR, BW, BY,	BZ, CA, CH,
CN, CO, CI	CU, CZ, DE, DK,	DM, DZ, EC, EE, EG, ES,	FI, GB, GD,
		IN, IS, JP, KE, KG, KP,	
		MD, MG, MK, MN, MW, MX,	
		RO, RU, SC, SD, SE, SG,	
		UG, US, UZ, VC, VN, YU,	
RW: BW. GH. GI	I. KE. LS. MW. MZ.	SD, SL, SZ, TZ, UG, ZM,	ZW, AM, AZ,
BY, KG, K	MD, RU, TJ, TM,	AT, BE, BG, CH, CY, CZ,	DE, DK, EE,

ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN,

TD, TG

US 2005113423 A1 20050526 US 2004-800022 20040312 EP 1601657 A1 20051207 EP 2004-720345 20040312

R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, PL, SK

PRIORITY APPLN. INFO.:

US 2003-453978P P 20030312 WO 2004-US7492 W 20040312

OTHER SOURCE(S):

MARPAT 141:296010

GI

$$\begin{array}{c} C \\ N-N \\ A \\ X \end{array} \qquad I \\ \begin{array}{c} H \\ N \\ HO \end{array} \qquad \qquad II \\ \end{array}$$

Pyrazoles I [A, B = (un) substituted aryl, heterocyclyl, cycloalkyl; C = H, AB (un) substituted aryl, heterocyclyl, heteroaryl, cycloalkyl, alkyl, alkylcarbonyl, arylcarbonyl, heteroarylcarbonyl, heterocyclylcarbonyl, or aminocarbonyl; X = H, (un) substituted alkyl, aryl, heterocyclyl, heteroaryl, or ω -substituted n-alkyl] such as II are prepared as inhibitors of ATP-binding cassette (ABC) transporters such as the cystic fibrosis transmembrane conductance regulator (CFTR) for use in the treatment of conditions such as cystic fibrosis, immunodeficiency, inflammatory disease, chronic obstructive pulmonary disease, chronic pancreatitis, or pneumonia. 4-Trifluoromethylbenzoyl chloride and 2-hydroxy-5-fluoroacetophenone are stirred in pyridine for 12 h, after which potassium hydroxide is added and the mixture stirred for 12 h; addition of hydrazine hydrate to a solution of the product obtained in the first step in ethanol and heating at reflux for 3 h yields II in 30% overall yield as a yellow crystalline solid. II modulates ∆F508-CFTR at ≥75% of the effect of genistein on the same receptor. Data on the relative modulation of Δ F508-CFTR by some compds. of the invention as compared to genistein is provided.

REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

=> file reg SINCE FILE TOTAL COST IN U.S. DOLLARS ENTRY SESSION 10.03 179.38 FULL ESTIMATED COST DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS) SINCE FILE TOTAL SESSION ENTRY -0.75 -0.75CA SUBSCRIBER PRICE

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STRUCTURE FILE UPDATES: 7 FEB 2006 HIGHEST RN 873775-18-9 DICTIONARY FILE UPDATES: 7 FEB 2006 HIGHEST RN 873775-18-9

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TSCA INFORMATION NOW CURRENT THROUGH JULY 14, 2005

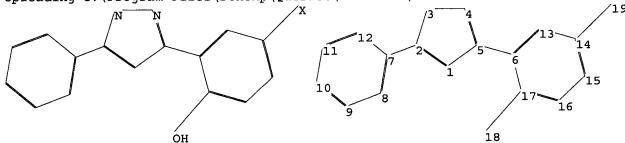
Please note that search-term pricing does apply when conducting SmartSELECT searches.

Structure search iteration limits have been increased. See HELP SLIMITS for details.

REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

http://www.cas.org/ONLINE/UG/regprops.html

Uploading C:\Program Files\Stnexp\Queries\10800022\Struc 4.str



chain nodes :
18 19
ring nodes :
1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17
chain bonds :
2-7 5-6 14-19 17-18
ring bonds :
1-2 1-5 2-3 3-4 4-5 6-13 6-17 7-8 7-12 8-9 9-10 10-11 11-12 13-14
14-15 15-16 16-17

exact/norm bonds :

1-2 1-5 2-3 3-4 4-5 17-18

exact bonds : 2-7 5-6 14-19 normalized bonds :

6-13 6-17 7-8 7-12 8-9 9-10 10-11 11-12 13-14 14-15 15-16 16-17

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:CLASS 19:CLASS

L9 STRUCTURE UPLOADED

=> d L9 HAS NO ANSWERS L9 STR

Structure attributes must be viewed using STN Express query preparation.

50 ANSWERS

=> 19

SAMPLE SEARCH INITIATED 14:49:26 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 1140 TO ITERATE

100.0% PROCESSED 1140 ITERATIONS INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**

PROJECTED ITERATIONS: 20775 TO 24825 PROJECTED ANSWERS: 1214 TO 2346

L10 50 SEA SSS SAM L9

=>

Uploading C:\Program Files\Stnexp\Queries\10800022\Struc 5.str

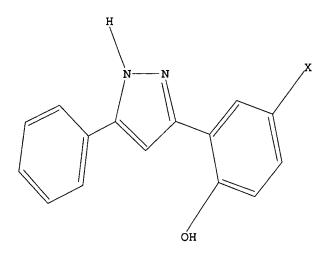
chain nodes :
18 19 20
ring nodes :
1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17
chain bonds :
2-7 3-20 5-6 14-19 17-18
ring bonds :
1-2 1-5 2-3 3-4 4-5 6-13 6-17 7-8 7-12 8-9 9-10 10-11 11-12 13-14
14-15 15-16 16-17
exact/norm bonds :
1-2 1-5 2-3 3-4 4-5 17-18
exact bonds :
2-7 3-20 5-6 14-19
normalized bonds :
6-13 6-17 7-8 7-12 8-9 9-10 10-11 11-12 13-14 14-15 15-16 16-17

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:CLASS 19:CLASS 20:CLASS

L11 STRUCTURE UPLOADED

=> d L11 HAS NO ANSWERS L11 STR



Structure attributes must be viewed using STN Express query preparation.

=> 111

SAMPLE SEARCH INITIATED 14:50:25 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 1140 TO ITERATE

100.0% PROCESSED 1140 ITERATIONS 3 ANSWERS

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 20775 TO 24825

PROJECTED ITERATIONS: 20775 TO 24825 PROJECTED ANSWERS: 3 TO 163

L12 3 SEA SSS SAM L11

=> 111 full

FULL SEARCH INITIATED 14:50:30 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 22881 TO ITERATE

100.0% PROCESSED 22881 ITERATIONS 43 ANSWERS

SEARCH TIME: 00.00.01

L13 43 SEA SSS FUL L11

=> file caplus

COST IN U.S. DOLLARS
SINCE FILE TOTAL
ENTRY SESSION
FULL ESTIMATED COST
169.58
348.96

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE
ENTRY
SESSION
CA SUBSCRIBER PRICE

0.00
-0.75

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FILE COVERS 1907 - 9 Feb 2006 VOL 144 ISS 7 FILE LAST UPDATED: 8 Feb 2006 (20060208/ED)

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http://www.cas.org/infopolicy.html

=> file medline caplus

COST IN U.S. DOLLARS SINCE FILE TOTAL ENTRY SESSION TULL ESTIMATED COST 0.46 349.42

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE
ENTRY
SESSION
CA SUBSCRIBER PRICE

0.00
-0.75

FILE 'MEDLINE' ENTERED AT 14:50:40 ON 09 FEB 2006

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=> 113

L14 11 L13

=> dup rem 114

PROCESSING COMPLETED FOR L14

L15 11 DUP REM L14 (0 DUPLICATES REMOVED)

=> d ibib abs hitstr 1-11

L15 ANSWER 1 OF 11 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2004:780671 CAPLUS

DOCUMENT NUMBER: 141:296010

TITLE: Preparation of substituted pyrazoles as modulators of

ATP-binding cassette transporters

INVENTOR(S): Vangoor, Frederick F.; Hadida Ruah, Sarah S.; Singh,

Ashvani K.; Olson, Eric R.; Makings, Lewis R.; Gonzalez, Jesus E., III; Rader, James A.; Chambers, Fred, III; Miller, Mark T.; Grootenhuis, Peter; Liu,

Yahua

PATENT ASSIGNEE(S): Vertex Pharmaceuticals Incorporated, USA

SOURCE: PCT Int. Appl., 174 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

		APPLICATION NO.	
		WO 2004-US7492	
W: AE, AG, AL,	AM, AT, AU, AZ,	BA, BB, BG, BR, BW,	BY, BZ, CA, CH,
CN, CO, CR,	CU, CZ, DE, DK,	DM, DZ, EC, EE, EG,	ES, FI, GB, GD,
GE, GH, GM,	HR, HU, ID, IL,	IN, IS, JP, KE, KG,	KP, KR, KZ, LC,
LK, LR, LS,	LT, LU, LV, MA,	MD, MG, MK, MN, MW,	MX, MZ, NA, NI,
		RO, RU, SC, SD, SE,	
		UG, US, UZ, VC, VN,	
		SD, SL, SZ, TZ, UG,	
		AT, BE, BG, CH, CY,	
		IT, LU, MC, NL, PL,	
		CM, GA, GN, GQ, GW,	
TD, TG	20, 61, 60, 61,	0, 0, 0, 0,	,,,
	71 20050526	US 2004-800022	20040312
		EP 2004-720345	
		GB, GR, IT, LI, LU,	
IE, SI, LT,	LV, FI, RO, MK,	CY, AL, TR, BG, CZ,	EE, HU, PL, SK
PRIORITY APPLN. INFO.:		US 2003-453978P	
		WO 2004-US7492	
OTHER SOURCE(S):	MARPAT 141:2960	10	

GI

$$C$$
 $N-N$
 B
 HO
 F
 II

Pyrazoles I [A, B = (un) substituted aryl, heterocyclyl, cycloalkyl; C = H, AΒ (un) substituted aryl, heterocyclyl, heteroaryl, cycloalkyl, alkyl, alkylcarbonyl, arylcarbonyl, heteroarylcarbonyl, heterocyclylcarbonyl, or aminocarbonyl; X = H, (un)substituted alkyl, aryl, heterocyclyl, heteroaryl, or ω -substituted n-alkyl] such as II are prepared as inhibitors of ATP-binding cassette (ABC) transporters such as the cystic fibrosis transmembrane conductance regulator (CFTR) for use in the treatment of conditions such as cystic fibrosis, immunodeficiency, inflammatory disease, chronic obstructive pulmonary disease, chronic pancreatitis, or pneumonia. 4-Trifluoromethylbenzoyl chloride and 2-hydroxy-5-fluoroacetophenone are stirred in pyridine for 12 h, after which potassium hydroxide is added and the mixture stirred for 12 h; addition of hydrazine hydrate to a solution of the product obtained in the first step in ethanol and heating at reflux for 3 h yields II in 30% overall yield as a yellow crystalline solid. II modulates ∆F508-CFTR at ≥75% of the effect of genistein on the same receptor. Data on the relative modulation of Δ F508-CFTR by some compds. of the invention as compared to genistein is provided. IT

148077-89-8P 148077-90-1P 296888-40-9P

immunodeficiency, and pneumonia)
RN 148077-89-8 CAPLUS

CN Phenol, 4-chloro-2-(5-phenyl-1H-pyrazol-3-yl)- (9CI) (CA INDEX NAME)

RN 148077-90-1 CAPLUS CN Phenol, 4-chloro-2-[5-(4-methoxyphenyl)-1H-pyrazol-3-yl]- (9CI) (CA INDEX NAME)

RN 296888-40-9 CAPLUS CN Phenol, 4-chloro-2-[5-(2-nitrophenyl)-1H-pyrazol-3-yl]- (9CI) (CA INDEX NAME)

RN 312518-98-2 CAPLUS CN Phenol, 4-chloro-2-[5-[4-(trifluoromethyl)phenyl]-1H-pyrazol-3-yl]- (9CI) (CA INDEX NAME)

RN 321534-47-8 CAPLUS CN Phenol, 4-chloro-2-[5-(4-fluorophenyl)-1H-pyrazol-3-yl]- (9CI) (CA INDEX NAME)

RN 423752-83-4 CAPLUS CN Phenol, 4-chloro-2-[5-[4-(1,1-dimethylethyl)phenyl]-1H-pyrazol-3-yl]-(9CI) (CA INDEX NAME)

RN 763132-68-9 CAPLUS CN Phenol, 4-fluoro-2-[5-[2-(trifluoromethyl)phenyl]-1H-pyrazol-3-yl]- (9CI) (CA INDEX NAME)

RN 763132-76-9 CAPLUS CN Phenol, 4-fluoro-2-[5-(2-nitrophenyl)-1H-pyrazol-3-yl]- (9CI) (CA INDEX NAME)

RN 763132-77-0 CAPLUS CN Phenol, 4-fluoro-2-(5-phenyl-1H-pyrazol-3-yl)- (9CI) (CA INDEX NAME)

RN 763133-02-4 CAPLUS

CN Phenol, 4-bromo-2-[5-(2-chlorophenyl)-1H-pyrazol-3-yl]- (9CI) (CA INDEX NAME)

RN 763133-77-3 CAPLUS

CN Phenol, 4-fluoro-2-[5-(2-fluorophenyl)-1H-pyrazol-3-yl]- (9CI) (CA INDEX NAME)

REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L15 ANSWER 2 OF 11 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2004:347011 CAPLUS

DOCUMENT NUMBER: 141:332110

TITLE: Design and synthesis of two pyrazole libraries based

on o-hydroxyacetophenones

AUTHOR(S): Borrell, Jose I.; Schuler, Elisabeth; Teixido, Jordi;

Michelotti, Enrique L.

CORPORATE SOURCE: Institut Quimic de Sarria, Grup d'Enginyeria

Molecular, Universitat Ramon Llull, Barcelona,

E-08017, Spain

SOURCE: Molecular Diversity (2004), 8(2), 147-157

CODEN: MODIF4; ISSN: 1381-1991

PUBLISHER: Kluwer Academic Publishers

DOCUMENT TYPE: Journal LANGUAGE: English

GI

Two new solid-phase syntheses of substituted pyrazoles are described. The first includes supporting an o-hydroxyacetophenone on Merrifield resin, Vilsmeier-Haack formylation on the Me group and cyclization with a substituted hydrazine to afford a pyrazole ring with two diversity centers, e.g. I [R1 = H, 4-F, 3,4-(MeO)2, etc., R2 = Ph, n-Pr, 2-benzothiazolyl, etc.]. The second starts from o-hydroxyacetophenone supported on Wang resin, which undergoes a Claisen condensation with a carboxylic acid ester to yield a 1,3-dicarbonyl compound that cyclizes to a pyrazole using a hydrazine, II and III (R = H, Me, Ph). Both methods have been used to synthesize two small pyrazole libraries.

IT 771483-26-2P 771483-38-6P 771483-49-9P

771483-53-5P

RL: CPN (Combinatorial preparation); CMBI (Combinatorial study); PREP (Preparation)

(design and solid-phase syntheses of pyrazole libraries using o-hydroxyacetophenones, their fungicidal, insecticidal, and herbicidal activities)

RN 771483-26-2 CAPLUS

CN Phenol, 4-chloro-2-(5-phenyl-1H-pyrazol-3-yl)-, mono(trifluoroacetate) (salt) (9CI) (CA INDEX NAME)

CM 1

CRN 148077-89-8 CMF C15 H11 Cl N2 O

CM 2

CRN 76-05-1 CMF C2 H F3 O2

RN 771483-38-6 CAPLUS
CN Phenol, 4-fluoro-2-(5-phenyl-1H-pyrazol-3-yl)-, mono(trifluoroacetate)
(salt) (9CI) (CA INDEX NAME)

CM 1

CRN 763132-77-0 CMF C15 H11 F N2 O

CM 2

CRN 76-05-1 CMF C2 H F3 O2

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Page 21
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RN 771483-49-9 CAPLUS
CN Phenol, 4-chloro-5-methyl-2-(5-phenyl-1H-pyrazol-3-yl)-,
mono(trifluoroacetate) (salt) (9CI) (CA INDEX NAME)

CM 1

CRN 487002-64-2
CMF C16 H13 C1 N2 O

CM 2

CRN 76-05-1 CMF C2 H F3 O2

RN 771483-53-5 CAPLUS
CN Phenol, 4-bromo-2-(5-phenyl-1H-pyrazol-3-yl)-, mono(trifluoroacetate)
(salt) (9CI) (CA INDEX NAME)

CM 1

CRN 121911-72-6 CMF C15 H11 Br N2 O

CM 2

CRN 76-05-1 CMF C2 H F3 O2

REFERENCE COUNT: 12 THERE ARE 12 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L15 ANSWER 3 OF 11 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2001:175150 CAPLUS

DOCUMENT NUMBER: 134:326294

TITLE: Synthetic analogs of naturally occurring flavolignans.

XI. Reaction of synthetic flavone analogs with

hydrazine hydrate and its derivatives

AUTHOR(S): Khilya, V. P.; Aitmambetov, A.; Kubzheterova, A.

CORPORATE SOURCE: Taras Shevchenko Kiev University, Ukraine

SOURCE: Chemistry of Natural Compounds (Translation of Khimiya

Prirodnykh Soedinenii) (2000), 36(1), 51-53

CODEN: CHNCA8; ISSN: 0009-3130

PUBLISHER: Consultants Bureau

DOCUMENT TYPE: Journal LANGUAGE: English

OTHER SOURCE(S): CASREACT 134:326294

AB Reactions of 1,3-benzodioxane and 1,4-benzodioxane analogs of flavones with hydrazine derivs. are studied. The hydrazines recyclize the new flavones into 3,5-diarylpyrazoles. Their PMR spectra confirm their structures.

IT 336612-27-2P 336612-33-0P 336612-34-1P

RL: SPN (Synthetic preparation); PREP (Preparation) (preparation of diarylpyrazoles via reaction of synthetic flavone analogs with hydrazine hydrate)

RN 336612-27-2 CAPLUS

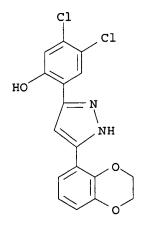
CN Phenol, 4-chloro-2-[5-(6-chloro-4H-1,3-benzodioxin-8-yl)-1H-pyrazol-3-yl]-(9CI) (CA INDEX NAME)

RN 336612-33-0 CAPLUS

CN Phenol, 2-[5-(2,3-dihydro-1,4-benzodioxin-5-yl)-1H-pyrazol-3-yl]-4-fluoro-(9CI) (CA INDEX NAME)

RN 336612-34-1 CAPLUS

CN Phenol, 4,5-dichloro-2-[5-(2,3-dihydro-1,4-benzodioxin-5-yl)-1H-pyrazol-3-yl]-(9CI) (CA INDEX NAME)



REFERENCE COUNT: 8 THERE ARE 8 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L15 ANSWER 4 OF 11 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1999:290178 CAPLUS

DOCUMENT NUMBER: 131:31901

TITLE: Synthesis of some new 4-iodoisoxazoles and -pyrazoles

and their antimicrobial activity

AUTHOR(S): Heda, P. B.; Ghiya, B. J.

CORPORATE SOURCE: Chemistry Department, Institute of Science, Nagpur,

440 001, India

SOURCE: Asian Journal of Chemistry (1999), 11(2), 384-387

CODEN: AJCHEW; ISSN: 0970-7077

PUBLISHER: Asian Journal of Chemistry

DOCUMENT TYPE: Journal LANGUAGE: English

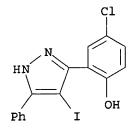
AB 1,3-Diaryl-1,3-propanediones were iodinated by iodine monochloride in dioxane to give 1,3-diaryl-2-iodo-1,3-propanediones, which were condensed with hydroxylamine hydrochloride, hydrazine hydrate, and phenylhydrazine in ethanol to give 4-iodo-3,5-diarylisoxazoles, 4-iodo-3,5-diarylpyrazoles, and 4-iodo-1,3,5-triarylpyrazoles, resp. The structures of the products were confirmed by elemental anal., chemical properties, and

IR, NMR, and mass spectral data. The antibacterial activity of some of the products was also studied.

IT 226877-80-1P

RN 226877-80-1 CAPLUS

CN Phenol, 4-chloro-2-(4-iodo-5-phenyl-1H-pyrazol-3-yl)- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L15 ANSWER 5 OF 11 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2000:92422 CAPLUS

DOCUMENT NUMBER: 132:265141

TITLE: Synthesis and reactions of 1,5-disubstituted-1,3-

propanediones

AUTHOR(S): Damle, Subhash V.; Muley, Prakash R.

CORPORATE SOURCE: Department of Chemistry, The Institute of Science,

Mumbai, 400 032, Russia

SOURCE: Indian Journal of Heterocyclic Chemistry (1999), 9(2),

81-86

CODEN: IJCHEI; ISSN: 0971-1627

PUBLISHER: Prof. R. S. Varma

DOCUMENT TYPE: Journal LANGUAGE: English

OTHER SOURCE(S): CASREACT 132:265141

GI

The title compds. I (R1 = H, Me; R2 = Cl, Me; R3 = 2-, 3-, 4-NO2; R4 = H, Cl, Me) have been synthesized by the base catalyzed Baker-Venkataraman transformation of esters of substituted 2-hydroxyacetophenones. Propanediones I on acid catalyzed cyclization afforded 2-(nitro-substituted phenyl)-4H-1-benzopyran-4-ones II (R1 = H, Me; R2 = Cl, Me; R3 = 2-, 3-, 4-NO2; R4 = H, Cl, Me). Condensation of I with hydrazine hydrate or phenylhydrazine afforded 3-(2-hydroxyphenyl)-5-(nitro-substituted phenyl)pyrazoles III (R1 = H; R2 = Cl, Me; R3 = 2-, 3-, 4-NO2; R4 = H, Cl, Me; R5 = H, Ph). Condensation of these propanediones with NH2OH.HCl in pyridine gave 3-(2-hydroxyphenyl)-5-(nitro-substituted phenyl)isoxazoles IV (R1 = H; R2 = Cl, Me; R3 = 2-, 3-, 4-NO2; R4 = H, Cl, Me), while in alc. the isomeric 3-(nitro-substituted phenyl)-5-(2-hydroxyphenyl)isoxazoles V were obtained.

IT 263364-40-5P 263364-41-6P 263364-42-7P

RL: SPN (Synthetic preparation); PREP (Preparation) (preparation of 1,5-disubstituted-1,3-propanediones from 2-hydroxyacetophenones and reactions to form benzopyranones, pyrazoles, and isoxazoles)

RN 263364-40-5 CAPLUS

CN Phenol, 2,4-dichloro-6-[5-(2-nitrophenyl)-1H-pyrazol-3-yl]- (9CI) (CA INDEX NAME)

RN 263364-41-6 CAPLUS

CN Phenol, 2,4-dichloro-6-[5-(3-nitrophenyl)-1H-pyrazol-3-yl]- (9CI) (CA INDEX NAME)

RN 263364-42-7 CAPLUS

CN Phenol, 2,4-dichloro-6-[5-(4-nitrophenyl)-1H-pyrazol-3-yl]- (9CI) (CA INDEX NAME)

REFERENCE COUNT:

8 THERE ARE 8 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L15 ANSWER 6 OF 11 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER:

1998:754850 CAPLUS

DOCUMENT NUMBER:

130:81452

TITLE:

Dehydrogenation of pyrazoline and its derivative using

10800022.trn

DMSO-I2-H2SO4 and DMSO-I2-system

AUTHOR(S): Raut, A. W.; Doshi, A. G.

CORPORATE SOURCE: Department of Chemistry, Shri Shivaji College,

Amravati, 444 602, India

SOURCE: Oriental Journal of Chemistry (1998), 14(2), 349-350

CODEN: OJCHEG; ISSN: 0970-020X

PUBLISHER: Oriental Scientific Publishing Co.

I

II

DOCUMENT TYPE: Journal LANGUAGE: English

GI

AB Pyrazolines I (R1 = H, Ac, Bz; R2 = H, MeO) were suspended in DMSO and a crystal of iodine added to it. The mixture was refluxed for 1 h, cooled, diluted with water, the solid obtained was filtered, washed with 20% aqueous sodium thiosulfate and crystallized from ethanol to give 75-82% pyrazoles II. The same reaction was carried out in DMSO-I2-H2SO4 system to give 72-78% pyrazoles II.

IT 218620-54-3P 218620-57-6P

RL: SPN (Synthetic preparation); PREP (Preparation) (dehydrogenation of pyrazolines using DMSO-I2-H2SO4 and DMSO-I2-system) 218620-54-3 CAPLUS

CN Phenol, 2-bromo-4-chloro-6-[5-(4-methoxyphenyl)-1H-pyrazol-3-yl]- (9CI) (CA INDEX NAME)

RN

RN 218620-57-6 CAPLUS

CN Phenol, 2-bromo-4-chloro-6-(5-phenyl-1H-pyrazol-3-yl)- (9CI) (CA INDEX NAME)

REFERENCE COUNT: 10 THERE ARE 10 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L15 ANSWER 7 OF 11 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1997:116095 CAPLUS

DOCUMENT NUMBER: 126:171535

TITLE: Structure-activity relationship studies of novel

pyrazolo(1,5-c][1,3]benzoxazines. Synthesis and

benzodiazepine receptor affinity

AUTHOR(S): Varano, Flavia; Catarzi, Daniela; Colotta, Vittoria;

Cecchi, Lucia; Filacchioni, Guido; Galli, Alessandro;

Costagli, Chiara

CORPORATE SOURCE: Dipartimento Scienze Farmaceutiche, Universita

Firenze, Florence, I-50121, Italy

SOURCE: Archiv der Pharmazie (Weinheim, Germany) (1996),

329(12), 529-534

CODEN: ARPMAS; ISSN: 0365-6233

PUBLISHER: VCH
DOCUMENT TYPE: Journal
LANGUAGE: English

GI

$$R^1$$
 N
 N
 N
 N
 N

AB Some pyrazolobenzoxazinones I (R = 2-FC6H4, 4-ClC6H4, 2-thienyl, CO2Et, CO2CHMe2, CO2Me; R1 = H, Cl) were prepared and were evaluated for their binding at benzodiazepine receptor (BZR) in rat cortical membranes. Structure-activity relationship studies suggest that, although proton donor d and proton acceptor al are both optional pharmacophoric descriptors, at least one of them must be present for good BZR affinity. When the proton donor d is not present, the heteroatom acceptor al is necessary either in the tricyclic core or in the appended substituent at the C(2) to obtain sub-micromolar BZR affinity.

IT 187173-72-4P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation, benzodiazepine receptor affinity, and structure-activity relationship of pyrazolobenzoxazines)

RN 187173-72-4 CAPLUS

CN Phenol, 4-chloro-2-[5-(2-fluorophenyl)-1H-pyrazol-3-yl]- (9CI) (CA INDEX NAME)

L15 ANSWER 8 OF 11 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1993:408806 CAPLUS

DOCUMENT NUMBER: 119:8806

TITLE: Preparation and biological activity of

3(5)-(hydroxyaryl)pyrazoles

INVENTOR(S): Kaestner, Gerd; Runge, Hans Joachim; Luecke, Lothar;

Loose, Sylva; Schewe, Christiane; Schewe, Tankred

PATENT ASSIGNEE(S): Chemische und Pharmazeutische Fabriken Fahlberg-List

G.m.b.H., Germany

SOURCE: Ger. Offen., 9 pp.

CODEN: GWXXBX

DOCUMENT TYPE: Patent

LANGUAGE: German

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 4126543 PRIORITY APPLN. INFO.:	A1	19930211	DE 1991-4126543 DE 1991-4126543	19910810 19910810
OTHER SOURCE(S):	MARPAT	119:8806		

AB The preparation of title compds. I (Ar = substituted 2-hydroxyphenyl; R = substituted alkyl, Ph, naphthyl; R1 = H, alkyl, cycloalkyl) as lipoxygenase and cyclooxygenase inhibitors and as well as antiasthmatic bronchodialators, inflammation inhibitors, allergy inhibitors, and skin disease treatment is claimed.

RN 121911-74-8 CAPLUS CN Phenol, 2,4-dichloro-6-(5-phenyl-1H-pyrazol-3-yl)- (9CI) (CA INDEX NAME)

RN 148077-89-8 CAPLUS CN Phenol, 4-chloro-2-(5-phenyl-1H-pyrazol-3-yl)- (9CI) (CA INDEX NAME)

RN 148077-90-1 CAPLUS CN Phenol, 4-chloro-2-[5-(4-methoxyphenyl)-1H-pyrazol-3-yl]- (9CI) (CA INDEX NAME)

L15 ANSWER 9 OF 11 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1991:61994 CAPLUS

DOCUMENT NUMBER: 114:61994

TITLE: Synthesis of new hydroxyarylpyrazolines and

chlorohydroxyarylpyrazoles of potential biological

activity

AUTHOR(S): Osman, S. A. M.; Hammad, M.; Swellem, R. H.;

El-Bayouki, K. A. M.

CORPORATE SOURCE: Natl. Res. Cent., Cairo, Egypt

SOURCE: Egyptian Journal of Chemistry (1989), Volume Date

1987, 30(6), 481-90

CODEN: EGJCA3; ISSN: 0367-0422

DOCUMENT TYPE: Journal LANGUAGE: English

OTHER SOURCE(S): CASREACT 114:61994

GΙ

Title pyrazolines I (R = Ph, 4-ClC6H4, 2-thienyl; R1=H, R2 = H, Cl) were prepared by the reaction of chalcones II with N2H4. Various derivs. of I (R1 = Ac, CONHPh) were also prepared by reacting I (R1 = H) with Ac2O and PhNCO resp. On refluxing in MeOH I (R = Ph, 4-ClC6H4; R1 = H, R2 = Cl) were oxidized to title pyrazoles III. Antimicrobial activity of I (R = Ph, 2-thienyl; R1 = H, Ac, CONHPh, CHO; R2 = H, Cl) and III (R = Ph, R1 = H, R2 = Cl) against various micro-organisms was tested. Most showed

general activity in concns. of 25-100 µg/mL.

IT 121911-74-8P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)

(preparation and bactericidal and fungicidal activity of)

RN 121911-74-8 CAPLUS

CN Phenol, 2,4-dichloro-6-(5-phenyl-1H-pyrazol-3-yl)- (9CI) (CA INDEX NAME)

IT 131557-38-5P

RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation of)

RN 131557-38-5 CAPLUS

CN Phenol, 2,4-dichloro-6-[5-(4-chlorophenyl)-1H-pyrazol-3-yl]- (9CI) (CA INDEX NAME)

L15 ANSWER 10 OF 11 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1989:477903 CAPLUS

DOCUMENT NUMBER: 111:77903

TITLE: Synthesis of some new 3,5-disubstituted-pyrazoles

AUTHOR(S): Ingle, V. N.

CORPORATE SOURCE: Dep. Chem., Nagpur Univ., Nagpur, 440 010, India

SOURCE: Journal of the Indian Chemical Society (1988), 65(12),

U

852

CODEN: JICSAH; ISSN: 0019-4522

DOCUMENT TYPE: Journal LANGUAGE: English

OTHER SOURCE(S): CASREACT 111:77903

GΙ

Cyclization of RCOCH2COR1 (R = Ph, p-anisyl, p-O2NC6H4; R1 = 2,3-, 2,4-, AΒ 2,5-HO(Me)C6H3, 2,5-HO(Br)C6H3, 2,3,4-HO(Me)2C6H2, 2,3,5-HO(Cl)2C6H2,

o-HOC6H4) with H2NNH2 gave 50-76% of 8 pyrazoles I.

IT 121911-72-6P 121911-74-8P

RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation of)

121911-72-6 CAPLUS RN

Phenol, 4-bromo-2-(5-phenyl-1H-pyrazol-3-yl)- (9CI) (CA INDEX NAME) CN

RN 121911-74-8 CAPLUS

Phenol, 2,4-dichloro-6-(5-phenyl-1H-pyrazol-3-yl)- (9CI) (CA INDEX NAME) CN

L15 ANSWER 11 OF 11 CAPLUS COPYRIGHT 2006 ACS on STN

1985:95573 CAPLUS ACCESSION NUMBER:

DOCUMENT NUMBER: 102:95573

Synthesis and antifungal activity of some TITLE:

1-substituted 3-(2-hydroxyphenyl)-5-(4-

nitrophenyl)pyrazoles

Giri, S.; Afshan, N., Mrs.; Nizamuddin AUTHOR(S):

Chem. Dep., Univ. Gorakhpur, Gorakhpur, India CORPORATE SOURCE:

Bokin Bobai (1984), 12(9), 437-40 SOURCE:

Journal

CODEN: BOBODP; ISSN: 0385-5201

DOCUMENT TYPE:

LANGUAGE: English GI

$$O_2C$$
 O_2C
 O_2C

AB RC6H3(OH)COMe-2,1 (R = 3-Me, 4-Me, 5-Cl, H) were treated with p-O2NC6H4CO2H and the resulting I underwent Baker-Venakataramam rearrangement to give the diketones II, which underwent cyclization with R1NHNH2 (R1 = H, Ph, 2,4-(O2N)2C6H3) to give the title compds. III. At 100 ppm III (R = 3-Me, R1 = H) inhibited Aspergillus niger by 60.9%.

IT 94951-49-2P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological

study); PREP (Preparation)
 (preparation and fungicidal activity of)

RN 94951-49-2 CAPLUS

CN Phenol, 4-chloro-2-[5-(4-nitrophenyl)-1H-pyrazol-3-yl]- (9CI) (CA INDEX NAME)

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(FILE 'HOME' ENTERED AT 14:42:11 ON 09 FEB 2006)

FILE 'REGISTRY' ENTERED AT 14:42:20 ON 09 FEB 2006
L1 STRUCTURE UPLOADED
L2 50 L1 '
L3 STRUCTURE UPLOADED
L4 0 L3

L5 STRUCTURE UPLOADED

L6 19 L5 L7 322 L5 FULL

FILE 'MEDLINE, CAPLUS' ENTERED AT 14:45:43 ON 09 FEB 2006

L8 1 L7

FILE 'REGISTRY' ENTERED AT 14:46:09 ON 09 FEB 2006

L9 STRUCTURE UPLOADED

L10 50 L9

L11 STRUCTURE UPLOADED

L12 3 L11

L13 43 L11 FULL

FILE 'CAPLUS' ENTERED AT 14:50:35 ON 09 FEB 2006

FILE 'MEDLINE, CAPLUS' ENTERED AT 14:50:40 ON 09 FEB 2006

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L15 11 DUP REM L14 (0 DUPLICATES REMOVED)

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